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LETTER TO THE EDITOR

Exact second-order correlation functions for random surface fractals

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Abstract. Exact analytical expressions for second-order correlation functions of both statistically homogeneous and heterogeneous models for random surface fractals are presented. The treatment is based on random germ–grain models and set-theoretical operations. The homogeneous two-phase models are variable with respect to volume fraction (0 to 1), fractal dimension of the internal surface (2 to 3) and the geometry of the convex grains. For heterogeneous models, the characteristics of two-phase microstructures superimposed onto the homogeneous fractal substructure can also be varied in a wide range.

The second-order correlation function $C(r)$ is an important characteristic of random two-phase structures. It describes the probability of finding two arbitrary test points, both situated within one of the two phases, and its dependence on the distance of the test points. Several physical properties are directly related to $C(r)$. One of these is the small-angle scattering intensity (see, for example, Glatter and Kratky (1982)), which is simply the Fourier transform of $C(r)$. Another property is the absorption behaviour of x-rays scattered by heterogeneous materials with non-vanishing absorption contrast (Hermann and Ermrich 1987).

In the present letter, the second-order correlation function $C(r)$ is derived for variable models of random surface fractals. The considered models are generalizations of the spherical tremata model proposed by Mandelbrot (1991), the homogeneous discrete scaling model by Hermann (1991a, b), and the continuous scaling model by Hermann and Ohser (1993). The generalizations concern the shape of the basic geometrical objects (grains) and the generation of two-phase microstructures, with fractal substructure of one phase. Exact expressions are given for $C(r)$, where the fractal dimension d_f of the internal surface is tunable in the complete range $2 < d_f < 3$, and the volume fraction c can also be chosen arbitrarily, i.e. $0 < c < 1$.

A series of models for fractal structures is based on numerical algorithms. One of these is the cluster–cluster aggregation model by Thouy and Jullien (1994), with tunable fractal dimension and analytical solutions for some special cases. The algorithms for the construction of the present models can, of course, also be realized on a computer. This should be performed if, for example, higher-order characteristics of the models are to be analysed.

The discrete and continuous scaling models mentioned above are based on random germ–grain algorithms. The germs are given by the points of a random-point field generated according to the well known Poisson distribution and characterized by the number density

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of points λ. Each of the germs is covered by a convex grain of size b, where overlaps of grains may occur. Then, a random set A is defined, comprising all grains distributed in this way. The surface of the random set A can be fractal or non-fractal, depending on the values of λ and the parameters of the size distribution of the grains. Volume fraction c_A and correlation function $C_A(r)$ of A are given (cf, for example, Stoyan *et al* (1987), Hermann (1991a)) by

$$c_A = 1 - \exp(-\lambda \bar{V}) \tag{1}$$

and

$$C_A(r) = 2c_A - 1 + (1 - c_A)^2 \exp[\lambda \bar{\gamma}(r)] \tag{2}$$

where $\bar{V}$ is the mean volume of the grains.

$$\bar{\gamma}(r) = \left\langle \left\langle \frac{1}{V} \int s(u+r)s(u)\,\mathrm{d}V_u \right\rangle_{\Omega} \right\rangle_{\text{grains}} \tag{3}$$

is the distance probability function of the grains averaged over all spatial orientations ($\langle\cdots\rangle_\Omega$) of a single grain and over all grains ($\langle\ldots\rangle_{\text{grains}}$), used for the construction of the model where a given grain is characterized by its shape function

$$s(r) = \begin{cases} 1 & r \in \text{grain} \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

The homogeneous continuous scaling model is defined by

$$A = \cup_{u=u_1}^{1} A_u \tag{5}$$

where A_u is a germ–grain model with parameters

$$\bar{b}_u = u^{\nu}\bar{b}_0 \qquad \lambda_u = u^{-\mu}\lambda_0 \qquad u_1 \leqslant u \leqslant 1. \tag{6}$$

For $u_1 \to 0$ and

$$2\nu + 1 \leqslant \mu \leqslant 3\nu + 1 \tag{7}$$

the model is fractal with

$$d_f = \frac{\mu - 1}{\nu}. \tag{8}$$

(The fractal dimension is calculated according to the Minkowski–Bouligand definition, see Zähle (1984), Hermann and Ohser (1993).) Now, $C_A(r)$ is calculated using random Poisson polyhedra as grains. (For definition and properties of Poisson polyhedra see Stoyan *et al* (1987).) A set of Poisson polyhedra is characterized by the mean breadth $\bar{b}_u$ (the breadth of a geometrical object is the distance between two parallel supporting planes; here, the average is taken over all spatial orientations of the measured object, and over all objects of the set), the mean volume

$$\bar{V}_u = \frac{16}{9\pi}\bar{b}_u^3 \tag{9}$$

and

$$\bar{\gamma}_u(r) = \bar{V}\exp(-3r/2\bar{b}_u). \tag{10}$$

Using (1), (5), (6) and the expressions

$$\lambda = \int_{u_1}^{1} \lambda_u \,\mathrm{d}u \tag{11}$$

$$\bar{V} = \int_{u_1}^{1} \frac{\lambda_u}{\lambda}\bar{V}_u \,\mathrm{d}u \tag{12}$$

$$\bar{\gamma}(r) = \int_{u_1}^{1} \frac{\lambda_u}{\lambda}\bar{\gamma}(r) \,\mathrm{d}u \tag{13}$$

and carrying out the limit $u_1 \to 0$, one obtains

$$\lambda\bar{\gamma}(r) = (3-d_f)\log\frac{1}{1-c_A}\int_0^1 x^{2-d_f}\exp(-3r/2\bar{b}_0 x)\,\mathrm{d}x \qquad r \geqslant 0 \tag{14}$$

$$= (3-d_f)\log\frac{1}{1-c_A}\left(\frac{3r}{2\bar{b}_0}\right)^{3-d_f}\{\Gamma(d_f-3)-\Gamma(d_f-3,0,3r/2\bar{b}_0)\}.$$

The homogeneous continuous scaling model with spherical grains can be treated analogously, where

$$\bar{\gamma}(r) = \frac{4\pi}{3}\int_{r/2}^{\infty} x^3\left(1-\frac{3r}{4x}+\frac{r^3}{16x^3}\right)f(x)\,\mathrm{d}x \tag{15}$$

must be used for averaging the distance probability function of the spheres, and $f(x)$ is the radii distribution (see, for example, Hermann (1991a)). Specifying $\bar{b}_0 = 2R_0$, where R_0 is the radius of the largest sphere, it follows that

$$\lambda\bar{\gamma}(r) = (3-d_f)\log\frac{1}{1-c_A}\left\{a_0 + a_1\frac{r}{\bar{b}_0} - a_2\left(\frac{r}{\bar{b}_0}\right)^3 - a_3\left(\frac{r}{\bar{b}_0}\right)^{3-d_f}\right\}$$

$$a_0 = \frac{1}{3-d_f} \qquad a_1 = \frac{3}{2}\frac{1}{d_f-2} \qquad a_2 = \frac{1}{2d_f} \qquad a_3 = a_0 + a_1 - a_2 \qquad 0 \leqslant r \leqslant \bar{b}_0. \tag{16}$$

Inserting, respectively, (14) and (16) into general expression (2) for the two-point correlation function of the used germ–grain models, one obtains $C_A(r)$ for homogeneous continuous scaling surface fractals with polyhedral and spherical grains. The model parameters are volume fraction c_A, $0 < c_A < 1$, maximum mean grain size $\bar{b}_0$, $\bar{b}_0 > 0$ and fractal dimension d_f, $2 < d_f < 3$.

The present surface fractals are homogeneous in a statistical sense. One can generate two-phase microstructures, where the substructure of one of the microstructural phases is fractal. Let

$$s_A(r) = \begin{cases} 1 & r \in A \\ 0 & \text{otherwise} \end{cases} \tag{17}$$

define the shape function of the homogeneous surface fractal A, and

$$s_M(r) = \begin{cases} 1 & r \in M \\ 0 & \text{otherwise} \end{cases} \tag{18}$$

the geometrical distribution M of the superimposed microstructural phase. The correlation function of the region $A \cap M$, which belongs to both A and M, is

$$C(r) = \frac{1}{V} \int s_A(u+r) s_A(u) s_M(u+r) s_M(u)\, dV_u \tag{19}$$

where the isotropy of the considered germ–grain models is taken into account, and M is also assumed to be isotropic.

Instead of M, one may choose a set M_ρ, which is obtained from M by shifting M by a vector ρ. Because of the statistical homogeneity of A, the characteristics of the fractal substructure in M and M_ρ are the same. Replacing M by M_ρ in (19), and averaging over ρ, one obtains

$$C(r) = C_A(r) C_M(r) \tag{20}$$

where $C_A(r)$ and $C_M(r)$ are the correlation functions of the statistically homogeneous surface fractal and phase M of the superimposed microstructure, respectively.

The variety of possible two-phase models, with fractal substructure of one of the phases, can even be extended by applying the set-theoretical operation

$$D \to D^c \tag{21}$$

where D^c is the set of all points outside D including the boundary of D. (D^c is called the complement of D.) Then, the relations

$$c_{D^c} = 1 - D^c \tag{22}$$

and

$$C_{D^c}(r) = C_D(r) + 1 - 2c_D \tag{23}$$

hold and can be used for further modifications of $C_A(r)$ and $C_M(r)$.

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